

Two-mode theory of BEC interferometry

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Abstract. A theory of BEC interferometry in an unsymmetrical double-well trap has been developed for small boson numbers, based on the two-mode approximation. The bosons are initially in the lowest mode of a single well trap, which is split into a double well and then recombined. Possible fragmentations into separate BEC states in each well during the splitting/recombination process are allowed for. The BEC is treated as a giant spin system, the fragmented states are eigenstates of S^2 and S_z . Self-consistent sets of equations for the amplitudes of the fragmented states and for the two single boson mode functions are obtained. The latter are coupled Gross-Pitaevskii equations. Interferometric effects may be measured via boson numbers in the first excited mode.

1 Introduction

The realization of Bose-Einstein condensates (BEC) in cold dilute atomic gases has opened up a new area of physics research on macroscopic quantum systems, since in a BEC at very low temperatures essentially all the bosons occupy the same single particle state (also referred to as modes or orbitals). Interference effects involving BECs were observed [1], [2], and there has been considerable interest in various schemes for constructing high precision interferometers using BECs [3], [4], [5]. Improvements in interferometer precision scaling as \sqrt{N} (where N is the number of bosons) may be possible [6]. Such interferometry is based on the similarity between the quantum states of BECs and those for lasers [7], in both cases a large number of bosons (atoms in one case, photons in the other) occupy a single mode, and hence BEC and laser interferometry is expected to be more precise than that based on single atoms or thermal light. The theoretical descriptions of the BEC and the laser are not quite the same of course. Laser light is often described in terms of coherent states (which are superpositions of number states), whereas in the BEC case descriptions based on number states are more appropriate, since superselection rules preclude superpositions of number states from being physical states [8]. In neither case however is the absolute phase of the laser or BEC state of any consequence for interferometry, indeed the idealized state of a single mode laser can be described by a density operator which involves a statistical mixture of coherent states with

all phases having equal weight, and therefore carries no more absolute phase information than the density operator for a number state that describes a BEC. Absolute phase is unimportant for interferometry because interference effects are associated with the relative phases between two or more contributions to certain total amplitudes whose moduli squared determine the measured effect - the interferometric effects are associated with the cross terms. There are many forms of interferometer, but both laser and BEC interferometers just involve particular ways of creating such interfering amplitudes. These amplitudes may have different natures - in an optical Mach-Zender interferometer a recombination of two electromagnetic field amplitudes associated with splitting the EM field into two different spatial pathways is involved, atomic Ramsey interferometers involve combining two quantum amplitudes for a transition that can take place via two different quantum pathways. The interpretation of the spatial interference patterns seen when two independent BECs are made to overlap involves considering the successive detection of bosons at various spatial positions [9], [10], [11], [12], [13], [14], and the interference pattern that builds up - which has a well-defined fringe spacing, but the absolute position of the fringes changes from one experiment to the next - is due to not knowing from which BEC any particular boson came. A well-defined relative phase is built up after many detections, and this is quite consistent with a fixed total boson number. Spatial interference effects based on successive boson detection can be described in terms of quantum correlation functions [15], [16], which in turn can be related to interfering quantum amplitudes.

Although in principle a BEC based atom interferometer should have similar advantages to a laser based optical interferometer, there are effects that could cause problems. Firstly, unlike photons bosons interact with each other, leading to non-linear terms in the Hamiltonian, and this causes dephasing effects that could destroy the interference patterns [17], [18]. Secondly, interactions with the environment, single boson thermal excitations, BEC collective excitations, soliton or vortex formation could also cause decoherence effects. Thirdly, although it is not necessary to prepare the bosons in a coherent state to produce interferometric effects, nor is it necessary to develop physical elements such as atomic mirrors or beam splitters in exact analogy to the optical case, an actual process must still be designed to produce some sort of interference effect that is reproducible from one experiment to the next - not all interference effects are useful for interferometry. Fourthly, single boson detection is not as well developed as single photon detection, and this makes BEC interferometry more difficult. Fifthly, since interferometry is used for conveniently measuring other quantities, it is desirable that the interferometric effect should be related to the quantity being measured via as simple a theory as possible.

The theory of single atom interferometers based on double well potentials is relatively simple [19], [20], [21], [22], and as interference of a BEC after splitting in a double well has been demonstrated [23], [24], a theory for BEC interferometers based on such double well potentials is of some interest, and this is the subject of the present paper. In addition, there is a considerable theo-

retical literature dealing with the behavior of BECs in double well potentials, describing effects such as self-trapping, Josephson oscillations, collapses and revivals of Bloch oscillations, macroscopic entanglement and so on (see [8], [25] for overviews). Many of these papers (see [26] and references therein) treat the BEC in a double well via various versions of a two-mode theory [27], and this suggests the idea of carrying out BEC interferometry in a regime where a simple two mode theory could be used to interpret the interferometric effects.

The proposed BEC interferometer involves the following process. Initially a large number N of bosons are at very low temperature and in the same spin state are trapped in a single potential well in a BEC state, with all the bosons in the lowest mode $\phi_1(r)$. This mode is essentially symmetric. The trapping potential is changed from a single well into a double well and back again over some suitable time scale. Experimentally this might involve magnetic traps on an atom chip consisting of permanent magnets plus current elements, the trap being changed by altering a bias field. The double well potential is in general asymmetric and this leads to interferometric effects, such as in the probability at the end of the interferometric process of bosons being found in the lowest excited mode $\phi_2(r)$, which is essentially antisymmetric. The asymmetry in the trapping potential may be due to gravitational effects for example, and the idea behind the interferometry is to detect such asymmetry effects by measuring the mean number of bosons found in the excited mode. The interferometer process is depicted in Figure 1.

As indicated above, the present work on double well BEC interferometry involves a simple theory based on the two-mode approximation. Decoherence, thermal, and multimode effects will be ignored and only restricted types of excitations and quantum fluctuations will be included. The theory is restricted to small boson numbers. Time dependent modes will be used to describe the adiabatic behavior, the dynamical behavior will involve amplitudes describing possible fragmented states of the N boson system. The system behaves like a giant spin system in the two-mode approximation. A variational approach involving spin operators will be used to determine self-consistent coupled equations for the amplitudes and modes, the latter equations being generalizations of the well-known Gross-Pitaevskii equation (GPE) [28], [29] used to describe a single BEC. The approach is a generalization based on papers by Menotti et al [30] and Spekkens et al [31], both of which use variational methods. Menotti et al [30] however restrict the modes and state amplitudes to be Gaussian forms parameterized by four variational functions, and coupled self-consistent equations are derived for these quantities. Dynamical BEC splitting, fragmentation, collapses and revivals are treated. Spekkens et al [31] use a variational principle and spin operator methods restricted to static, symmetrical potential cases to derive self-consistent coupled equations for state amplitudes and modes - giving generalized time independent Gross-Pitaevskii equations. Static BEC fragmentation is found. Cederbaum et al [32] predict fragmented excited BEC states in the static case using generalized time independent GPE derived using variational methods, but restricting fragmentation to a single choice of a 50:50 split

between the two wells. Numerous other papers (see [26] and references therein) have treated BEC dynamics in a double well potential, many either assuming fixed modes or that no BEC fragmentation occurs. Spin operators based on fixed modes have also been widely used.

The physics of the double well BEC interferometer based on a two mode treatment will be discussed in section 2. The theory of the interferometer, giving the self-consistent coupled equations for amplitudes of possible fragmented states and for the generalized Gross-Pitaevskii equations for the two single boson mode functions is presented in section 3. Considerations for numerical studies based on the coupled amplitude and mode equations are covered in section 4, and the paper is summarized in section 5. Detailed quantities involved in the basic equations are set out in the appendix.

2 Physics of double well BEC interferometry

The behavior of the double well BEC interferometer involves a number of important issues:

1. Does the BEC fragment into two BECs (left well, right well) during the process?
2. What happens to the single boson modes $\phi_1(r, t), \phi_2(r, t)$, as the trap potential changes?
3. What is the essential nature of the interferometric process involved?
4. What excited BEC states are important in the process?
5. What effect would decoherence, quantum fluctuations, finite temperatures, .. have?
6. How are the interferometric measurements, such as the excited boson probability, related to asymmetry in the trapping potential?
7. How does the interferometer sensitivity depend on the number of bosons?
8. What is the optimum way to change the trap potential during the process?

2.1 Fragmentation

The possibility of the BEC fragmenting into two parts - with some bosons being in one mode and the rest in a second mode (see [8], [25]) - can be seen if we consider the energy eigenstates for N bosons in a symmetric double well potential (see figure 2). To discuss this case we may consider two harmonic oscillator wells with frequency ω_0 separated by $2d$ as representing the two separate wells, with the actual double well having a barrier height V_B . Localized states $\phi_L(r)$ and $\phi_R(r)$ in each well, associated with annihilation operators \widehat{a}_L and \widehat{a}_R can

be introduced. For simplicity the extra effects due to double well asymmetry will be ignored at present, though of course some effects due to boson-boson interactions are included.

An approximate theoretical treatment can be based on the Bose-Hubbard Hamiltonian - a simple model for the N boson system

$$\begin{aligned}\hat{H}_{BH} = & -\frac{J}{2}(\hat{a}_R^\dagger \hat{a}_L + \hat{a}_L^\dagger \hat{a}_R) \\ & + \frac{U}{2}(\hat{n}_L\{\hat{n}_L - 1\} + \hat{n}_R\{\hat{n}_R - 1\}),\end{aligned}\quad (1)$$

where

$$J = -2 \int d\mathbf{r} \phi_L(\mathbf{r})^* \left(-\frac{\hbar^2}{2m} \nabla^2 + V\right) \phi_R(\mathbf{r}) \quad (2)$$

$$U = g \int d\mathbf{r} |\phi_L(\mathbf{r})|^4 \quad (3)$$

are the tunneling and boson-boson interaction parameters. It is well-known [8] that there are two regimes - the Josephson regime when $J \gg U$ and the Fock regime when $U \gg J$.

In the Josephson regime the ground state is given by

$$|\Phi_{BEC}\rangle = \frac{(\hat{a}_L^\dagger + \hat{a}_R^\dagger)^N}{(2)^{\frac{N}{2}} (N!)^{\frac{1}{2}}} |0\rangle \quad (4)$$

$$E_{BEC} = -\frac{1}{2} J N + \frac{1}{4} U N (N - 1). \quad (5)$$

In this case all N bosons are in the same delocalized state $(\phi_L + \phi_R)/\sqrt{2}$. This represents a single unfragmented condensate - the BEC phase.

In the Fock regime the ground state is given by

$$|\Phi_{MOTT}\rangle = \frac{(\hat{a}_L^\dagger)^{\frac{N}{2}} (\hat{a}_R^\dagger)^{\frac{N}{2}}}{(\frac{N}{2}!)^{\frac{1}{2}} (\frac{N}{2}!)^{\frac{1}{2}}} |0\rangle \quad (6)$$

$$E_{MOTT} = \frac{1}{4} U N (N - 2). \quad (7)$$

In this case the two localized states ϕ_L and ϕ_R are each occupied by $N/2$ bosons. This represents a fragmented condensate - the Mott phase.

Estimates based on harmonic oscillator wave functions

$$\phi_{L,R}(\mathbf{r}) = \left(\frac{1}{\pi a_0^2}\right)^{3/4} \exp\left(-\frac{(x \pm d)^2}{2 a_0^2}\right) \exp\left(-\frac{(y^2 + z^2)}{2 a_0^2}\right) \quad (8)$$

$$a_0 = \left(\frac{\hbar}{m\omega_0}\right)^{1/2} \quad g = \frac{4\pi\hbar^2 a_S}{m}, \quad (9)$$

gives

$$\frac{J}{U} \sim \frac{V_B}{\hbar\omega_0} \frac{a_0}{a_s} \exp\left(-\frac{d^2}{a_0^2}\right). \quad (10)$$

For Rb⁸⁷ with $a_s = 5$ nm, $a_0 = 1$ μ m, $\omega_0 = 2\pi \cdot 58$ s⁻¹, $V_B/\hbar\omega_0 = 10$, we find $J/U \sim 10^{-7}$ for $2d = 10$ μ m and $J/U \sim 10^{+2}$ for $2d = 4$ μ m. Thus both the Fock and Josephson regimes are accessible. Hence if the interferometric process is adiabatic, then either a single BEC or two fragmented BECs could be accessed depending on the double well parameters. On the other hand if the process is fast, then not all adiabatic states may be accessed. For specific double well parameters, whether the fragmentation occurs or not will thus depend on the time scale of the interferometer process. The effects of asymmetry in the trapping potential and of more general boson-boson interactions also need to be taken into account, but whether fragmentation effects occur or not cannot be just arbitrarily assumed.

2.2 Nature of Modes

Since the trapping potential changes from a single well to a double well and back again we expect the mode functions to change during the process, and if the process was done very slowly the notion of time dependent mode functions determined via a suitable adiabatic principle is a natural one. The question is - what form are the time dependent mode functions likely to have? For simplicity the extra effects due to boson-boson interactions will be ignored at present, though of course effects due to double well asymmetry are included. The possibilities for the situation where boson-boson interactions are unimportant can be seen by just solving the time dependent energy eigenvalue equations [22], and typical results are illustrated in Figure 3.

The situation for the single well regime is shown in Figure 3a. Here an approximately symmetric lowest energy eigenfunction and an approximately antisymmetric lowest excited energy eigenfunction occurs, corresponding to mode functions at the beginning and end of the interferometer process

In the middle of the interferometer process where a double asymmetric well regime occurs, two qualitatively different outcomes may occur. The two lowest mode functions may be approximately symmetric and antisymmetric functions which are delocalized over both wells. This case is shown in Figure 3b, and applies to situations where the asymmetry is small. On the other hand, if the asymmetry is larger, the two lowest mode functions are localized in different wells, and no longer are approximately symmetric or antisymmetric. This case is shown in Figure 3c. Thus, the nature of the mode functions will depend the trapping potential parameters, especially on the asymmetry of the double well. The effects of boson-boson interaction also must be taken into account, and as in the case of whether fragmentation effects occur or not, the form of the mode functions cannot be just arbitrarily assumed.

2.3 Interferometry Process

Essentially, the interferometric process from $t = 0$ to $t = T$ involves an initial state $|N, 0, 0\rangle$ and a final state $|N - n, n, T\rangle$ representing the transfer of n bosons from the first mode to the second (where in general $|N - m, m, t\rangle$ is a state at time t with $N - m$ bosons in mode $\phi_1(r, t)$ and m bosons in mode $\phi_2(r, t)$). The probability amplitude $A(n, T)$ for the process is related to the transition probability via $P(n, T) = |A(n, T)|^2$ and can be written in terms of time evolution operators $\hat{U}(t_2, t_1)$ as

$$A(n, T) = \langle N - n, n, T | \hat{U}(T, 0) | N, 0, 0 \rangle \quad (11)$$

$$= \sum_m \langle N - n, n, T | \hat{U}(T, T/2) | N - m, m, T/2 \rangle \\ \times \langle N - m, m, T/2 | \hat{U}(T/2, 0) | N, 0, 0 \rangle, \quad (12)$$

where the transitive property of the evolution operator has been used and a completeness relationship involving states at time $t = T/2$ has been inserted. The last expression (12) for the transition amplitude shows it to be the sum of contributions at the intermediate time $T/2$, where m bosons have been transferred from mode $\phi_1(r, 0)$ to mode $\phi_2(r, T/2)$. Clearly, quantum interference in the overall transition amplitude is present, with constructive or destructive interference possible. In this simple exposition there are N possible quantum pathways present, but if the time interval between $t = 0$ and $t = T$ is divided into a large number of steps, the number of pathways is hugely increased. Figure 4 illustrates the case where $N = 9$ and $n = 1$ boson is transferred into mode $\phi_2(r, T)$. Here there are two quantum pathways, one where the transfer of the boson occurs between $t = 0$ and $t = T/2$ and the other where it occurs between $t = T/2$ and $t = T$. The intermediate mode functions $\phi_i(r, T/2)$ are shown as localized modes, so the two intermediate states would then involve different numbers of bosons in the two wells.

2.4 Excited states, decoherence, finite temperatures and quantum fluctuations

Within the two-mode approximation, the basis states which can occur are limited to fragmented states in which some of the N bosons occupy the first mode $\phi_1(r, t)$ and the rest occupy the second mode $\phi_2(r, t)$. Although superpositions of such states (see equations (31), (34)) can be used to describe single BEC states where the mode is a superposition of $\phi_1(r, t)$ and $\phi_2(r, t)$ - and such states with all bosons in one mode might be approximations to a collective excited state of the BEC - the number of collective excited states that could be described this way is small, yet it is known that trapped BECs have a whole spectrum of collective excited states (see [25], [33]). Also, thermally excited states in which some of the bosons occupy further modes $\phi_3(r, t)$, $\phi_4(r, t)$, ..are also outside the scope of two-mode theory. Hence the two-mode theory does not allow for

multi-mode effects or all possible excited states that might be accessed during the interferometer process, especially if the initial temperature was a significant fraction of the BEC transition temperature.

Decoherence effects due to coupling with an external environment, or due to interactions between the BEC state and a continuum of thermally excited states, or due to fluctuations in the trapping potentials require treatments involving master equations and density operators, and this is also outside the scope of the pure state treatment presented here. A full theory of BEC interferometry taking into account excited states (collective and single particle), decoherence, finite temperatures, multi-mode effects and without restrictions on the boson number would be a worthwhile development. Such a theory could be based on phase space methods [34], in which the bosonic field operator is represented by a stochastic space-time function, the mean value of which resembles a condensate wave function. The stochastic condensate wave function satisfies a partial differential equation which contains noise terms due to quantum fluctuations and deterministic terms resembling those in a Gross-Pitaevskii equation. Alternatively, a full treatment of BEC interferometry could be based on Bogoliubov theory [35].

2.5 Interferometric measurements, sensitivity and optimum process

Several possible interferometric effects could be measured for the double well BEC interferometer, including the number of bosons ending up in the excited mode $\phi_2(r, T)$ or the final spatial boson density. The objective is to find which responds most sensitively to the other quantities (such as gravitational fields) that the interferometry is intended to measure, and this can only be determined via numerical studies of the operation of the interferometer. Such studies will include varying the parameters describing the process, such as the time scales, barrier heights, separation of the double wells, boson numbers and so on, to maximize the interferometric effects.

3 Theory

In terms of bosonic field operators $\hat{\Psi}(\mathbf{r}), \hat{\Psi}^\dagger(\mathbf{r})$ the Hamiltonian is given by

$$\hat{H} = \int d\mathbf{r} \left(\frac{\hbar^2}{2m} \nabla \hat{\Psi}^\dagger \cdot \nabla \hat{\Psi} + \hat{\Psi}^\dagger V \hat{\Psi} + \frac{g}{2} \hat{\Psi}^\dagger \hat{\Psi}^\dagger \hat{\Psi} \hat{\Psi} \right) \quad (13)$$

The first term represents the kinetic energy of the bosons each of which has mass m , the second term involves the time-dependent trapping potential $V(\mathbf{r}, t)$ and the third term allows for the two-body interaction between the bosons in the usual zero-range approximation. The coupling constant g is determined from the scattering length a_s via $g = 4\pi a_s \hbar^2 / m$. Since a single component BEC is involved only one pair of field operators is required.

The field operators satisfy the usual bosonic commutation rules

$$\left[\widehat{\Psi}(\mathbf{r}), \widehat{\Psi}^\dagger(\mathbf{r}')\right] = \delta(\mathbf{r} - \mathbf{r}') \quad (14)$$

Time dependent single boson mode functions $\phi_i(\mathbf{r}, t)$ will be used, chosen to be orthogonal and normalized at all times.

$$\int d\mathbf{r} \phi_i^*(\mathbf{r}, t) \phi_j(\mathbf{r}, t) = \delta_{ij} \quad (15)$$

The conditions in equation (15) for each time t will act as constraints in the variational method used to obtain equations for the two mode functions.

The field operators are expanded in terms of the mode functions, which introduces the mode annihilation $\widehat{c}_i(t)$ and creation operators $\widehat{c}_i^\dagger(t)$ as the time dependent operator expansion coefficients, the mode functions carrying all the position dependence. The creation and annihilation operators satisfy the standard bosonic commutation rules at all times.

$$\widehat{\Psi}(\mathbf{r}) = \sum_{i=1,2} \widehat{c}_i(t) \phi_i(\mathbf{r}, t) \quad \widehat{\Psi}^\dagger(\mathbf{r}) = \sum_{i=1,2} \widehat{c}_i^\dagger(t) \phi_i^*(\mathbf{r}, t) \quad (16)$$

$$\left[\widehat{c}_i(t), \widehat{c}_j^\dagger(t)\right] = \delta_{ij} \quad (i, j = 1, 2, \dots) \quad (17)$$

In the two-mode approximation only two terms are included in the expansions for the field operators.

The boson number operator \widehat{N} is defined by a space integral involving the field operators and may be also expressed as a sum involving mode annihilation and creation operators. Thus:

$$\widehat{N} = \int d\mathbf{r} \widehat{\Psi}^\dagger(\mathbf{r}) \widehat{\Psi}(\mathbf{r}) \quad (18)$$

$$= \sum_i \widehat{c}_i^\dagger \widehat{c}_i \quad (19)$$

The boson number is a conserved quantity and only state vectors with a single boson number N will be considered here. For convenience N will be even.

In a two-mode theory it is convenient to introduce spin operators defined by

$$\begin{aligned} \widehat{S}_x &= (\widehat{c}_2^\dagger \widehat{c}_1 + \widehat{c}_1^\dagger \widehat{c}_2)/2 \\ \widehat{S}_y &= (\widehat{c}_2^\dagger \widehat{c}_1 - \widehat{c}_1^\dagger \widehat{c}_2)/2i \\ \widehat{S}_z &= (\widehat{c}_2^\dagger \widehat{c}_2 - \widehat{c}_1^\dagger \widehat{c}_1)/2 \end{aligned} \quad (20)$$

The spin operators \widehat{S}_α satisfy the standard commutation rules for angular momentum operators

$$\left[\widehat{S}_\alpha, \widehat{S}_\beta\right] = i \epsilon_{\alpha\beta\gamma} \widehat{S}_\gamma \quad (\alpha, \beta, \gamma = x, y, z), \quad (21)$$

and the square of the angular momentum $(\hat{S})^2$ can be related to the boson number operator. Thus:

$$(\hat{S})^2 = \sum_{\alpha} (\hat{S}_{\alpha})^2 \quad (22)$$

$$= \frac{\hat{N}}{2} (\frac{\hat{N}}{2} + 1) \quad (23)$$

Clearly the angular momentum squared is a conserved quantity.

A set of states for the N boson system can be defined by

$$|k\rangle = \frac{(\hat{c}_1^\dagger)^{(\frac{N}{2}-k)} (\hat{c}_2^\dagger)^{(\frac{N}{2}+k)}}{[(\frac{N}{2}-k)!]^{\frac{1}{2}} [(\frac{N}{2}+k)!]^{\frac{1}{2}}} |0\rangle \quad (k = -N/2, -N/2 + 1, \dots, +N/2) \quad (24)$$

In general this represents a state with $(\frac{N}{2} - k)$ bosons in mode $\phi_1(r, t)$ and $(\frac{N}{2} + k)$ bosons in mode $\phi_2(r, t)$. Such a state is a fragmented state of the N boson system, involving two BECs not just one. These states will be used as orthogonal, normalized basis states for representing a general state of the bosonic system during the interferometer process. For the cases where $k = \pm N/2$ the N bosons are all in the same mode, so that an unfragmented single BEC is represented. Thus with $k = -N/2$ we have

$$\left| -\frac{N}{2} \right\rangle = \frac{(\hat{c}_1^\dagger)^N}{[N!]^{\frac{1}{2}}} |0\rangle. \quad (25)$$

This state is a single unfragmented BEC with all bosons in mode $\phi_1(r, t)$.

The N boson system behaves like a giant spin system in the two-mode approximation. The basis states $|k\rangle$ are simultaneous eigenstates of $(\hat{S})^2$ and \hat{S}_z with eigenvalues $\frac{N}{2}(\frac{N}{2} + 1)$ and k . Thus:

$$(\hat{S})^2 |k\rangle = \frac{N}{2} (\frac{N}{2} + 1) |k\rangle \quad (26)$$

$$\hat{S}_z |k\rangle = k |k\rangle. \quad (27)$$

Hence $j = \frac{N}{2}$ is the spin angular momentum quantum number, and k is the spin magnetic quantum number, with $(-\frac{N}{2} \leq k \leq \frac{N}{2})$. Thus the boson number N and the quantity k that specifies the fragmentation of the BEC between the two modes have a physical interpretation in terms of angular momentum theory. Since boson numbers may be $\sim 10^8$ the spin system is on a macroscopic scale. To emphasize the spin character of the basis states we can introduce the notation

$$|k\rangle \equiv \left| \frac{N}{2}, k \right\rangle \quad (28)$$

The methods of angular momentum theory can be utilized by first writing the Hamiltonian in terms of spin operators using equations (16), (20), and

its matrix elements calculated using angular momentum theory from previous expressions plus

$$\hat{S}_{\pm} \left| \frac{N}{2}, k \right\rangle = \left\{ \frac{N}{2} \left(\frac{N}{2} + 1 \right) - k(k \pm 1) \right\}^{\frac{1}{2}} \left| \frac{N}{2}, k \pm 1 \right\rangle \quad (29)$$

$$\hat{S}_{\pm} = \hat{S}_x \pm i\hat{S}_y. \quad (30)$$

The quantum state $|\Phi(t)\rangle$ of the N boson system during the interferometer process will be written as a superposition of the fragmented states $|k\rangle$, where the amplitude for this fragmented state is $b_k(t)$.

$$|\Phi(t)\rangle = \sum_{k=-\frac{N}{2}}^{\frac{N}{2}} b_k(t) |k\rangle. \quad (31)$$

Normalization of the state vector requires that the amplitudes satisfy the condition

$$\sum_{k=-\frac{N}{2}}^{\frac{N}{2}} |b_k(t)|^2 = 1, \quad (32)$$

which represents conservation of probability. The condition in equation (32) for each time t will act as constraints in the variational method used to obtain equations for the amplitudes. The initial condition involves having a single BEC with all bosons in mode $\phi_1(r, 0)$, thus:

$$|\Phi(0)\rangle = \left| -\frac{N}{2} \right\rangle \quad (33)$$

The form of the state vector given in equation (31) involves a physical assumption in that only the two mode fragmented states are included in the quantum superposition. This amounts to ignoring other possible states for the bosonic system, such as where bosons occupy more than two modes or where collective excited states such as breathing modes are involved. Further development of the theory to allow for the presence such other states may be required if the present simple approach proves inadequate.

It should be noted that as well as allowing for the possibility of fragmentation of the BEC into two modes, the state vector in equation (31) is also consistent with the situation where all N bosons are in a single mode of the form

$$\tilde{\phi}_1 = \cos \theta \exp(-i\frac{1}{2}\chi) \phi_1 + \sin \theta \exp(+i\frac{1}{2}\chi) \phi_2,$$

where θ determines the relative contributions from the original modes ϕ_1 and ϕ_2 , and where χ is a phase variable. In this case the amplitudes b_k are related to binomial coefficients and are given by

$$b_k = \left[\frac{N!}{(\frac{N}{2} - k)!(\frac{N}{2} + k)!} \right]^{\frac{1}{2}} (\cos \theta)^{\frac{N}{2} - k} (\sin \theta)^{\frac{N}{2} + k} \exp(-ik\chi). \quad (34)$$

This situation amounts to replacing the two mode functions ϕ_1, ϕ_2 by $\tilde{\phi}_1, \tilde{\phi}_2$ (where $\tilde{\phi}_2 = -\sin\theta \exp(-i\frac{1}{2}\chi) \phi_1 + \cos\theta \exp(+i\frac{1}{2}\chi) \phi_2$). The state vector is then given by an expression analogous to equation (24) with $k = -N/2$, but with the original creation operators $\hat{c}_1^\dagger, \hat{c}_2^\dagger$ replaced by new creation operators associated with the new modes $\tilde{\phi}_1, \tilde{\phi}_2$. If it turns out that the BEC does not fragment then the solutions for the amplitudes b_k will be in a form given by equation (34). Such states with all bosons in one mode might approximately represent a collective excited state of the BEC.

The amplitudes $b_k(t)$ and the mode functions $\phi_i(\mathbf{r}, t)$ can then be related to the various types of interferometer measurement. For example, the number of bosons in the mode $\phi_2(r, t)$ is given by

$$N_2 = \langle \Phi(t) | \hat{c}_2^\dagger(t) \hat{c}_2(t) | \Phi(t) \rangle \quad (35)$$

$$= \frac{N}{2} + \sum_k k |b_k|^2. \quad (36)$$

The time dependence is left understood in the result. Measurement of N_2 at end of the process depends on the asymmetry and exhibits interferometric effects because the probability amplitude at the end of the process for fragmented states with $k \neq -N/2$ in which there are bosons in the mode $\phi_2(r, t)$ will contain contributions from many quantum pathways. Interferometric effects of the spatial type can be described in terms of quantum correlation functions [15], [16]. For example, the first order correlation function is given by

$$G^{(1)}(\mathbf{r}, \mathbf{r}', t) = \langle \Phi(t) | \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}') | \Phi(t) \rangle \quad (37)$$

$$\begin{aligned} &= \sum_k b_k^* b_k \left\{ \phi_1(\mathbf{r})^* \phi_1(\mathbf{r}') \left(\frac{N}{2} - k \right) + \phi_2(\mathbf{r})^* \phi_2(\mathbf{r}') \left(\frac{N}{2} + k \right) \right\} \\ &\quad + \sum_k b_k^* b_{k+1} \left\{ \phi_1(\mathbf{r})^* \phi_2(\mathbf{r}') \sqrt{\left(\frac{N}{2} - k \right) \left(\frac{N}{2} + k + 1 \right)} \right\} \\ &\quad + \sum_k b_k^* b_{k-1} \left\{ \phi_2(\mathbf{r})^* \phi_1(\mathbf{r}') \sqrt{\left(\frac{N}{2} + k \right) \left(\frac{N}{2} - k + 1 \right)} \right\} \end{aligned} \quad (38)$$

where in the result the time dependence is left understood. More complex expressions are involved for the second order correlation function. The presence of spatial interferometric patterns and the existence of long range order in BECs can be determined from such correlation functions.

The equations governing the amplitudes $b_k(t)$ are obtained from a variational principle based on the dynamical action S_{dyn} . This quantity is a functional of quantum state $|\Phi(t)\rangle$ and is defined by

$$S_{dyn} = \int dt \left(\{ \langle \partial_t \Phi | \Phi \rangle - \langle \Phi | \partial_t \Phi \rangle \} / 2i - \langle \Phi | \hat{H} | \Phi \rangle / \hbar \right). \quad (39)$$

The Principle of Least Action involves the minimization of the action S_{dyn} for arbitrary variations of the state vector and this results in $|\Phi(t)\rangle$ satisfying the time-dependent Schrodinger equation (TDSE). The variations of the state vector are subject to the constraint that it remains normalized to unity. This variational principle may be regarded as the fundamental principle of quantum dynamics, so its application to a specific case such as the BEC interferometry process is on firm ground. In the present situation the state vector is restricted in its possible variations to remaining in the form given in equation (31) (though remaining normalized to unity), and hence does not itself satisfy the TDSE. What is obtained is a state vector which is an approximate solution to the TDSE, and it turns out that the amplitudes $b_k(t)$ involved in the form for the state vector could also be obtained by just assuming that $|\Phi(t)\rangle$ satisfied the TDSE. The present variational approach has been applied in many other quantum physics problems - the derivation of the time-dependent Hartree-Fock equations for electrons in an atom being one example. It has already been applied to BEC problems by Menotti et al [30], who described the amplitudes via a Gaussian function with two variational parameters.

For fixed modes $\phi_i(r, t)$ the action S_{dyn} is a functional of the amplitudes $b_k(t)$. The normalization constraint in equation (32) for time τ may be written in terms of the functional $F_\tau[b_k, b_k^*]$, which is required to equal unity. Thus

$$F_\tau[b_k, b_k^*] = \int dt \sum_l b_l^*(t) b_l(t) \delta(t - \tau) = 1. \quad (40)$$

The action S_{dyn} is minimized for arbitrary variation of the amplitudes subject to the normalization constraints, which are taken into account with Lagrange multipliers $\lambda(\tau)/\hbar$. In applying the Principle of Least Action, the functional derivatives of the action S_{dyn} plus the integral of the constraints F_τ each weighted with Lagrange multipliers $\lambda(\tau)/\hbar$ are equated to zero. Thus we have:

$$\frac{\delta}{\delta b_k^*} \Delta S_{dyn}[b_k, b_k^*] = \frac{\delta}{\delta b_k} \Delta S_{dyn}[b_k, b_k^*] = 0 \quad (41)$$

$$\Delta S_{dyn}[b_k, b_k^*] = S_{dyn}[b_k, b_k^*] + \int d\tau \frac{\lambda(\tau)}{\hbar} F_\tau[b_k, b_k^*] \quad (42)$$

It turns out that the Lagrange multiplier $\lambda(\tau)$ associated with the normalization constraint can be transformed away and need not appear in the equations for the amplitudes. The key equations for the amplitudes $b_k(t)$ are given below in equation (47).

The equations governing the mode functions $\phi_i(r, t)$ are also obtained from a variational principle, but now based on the adiabatic action S_{adia} . This quantity is a functional of quantum state $|\Phi(t)\rangle$ which is defined by

$$S_{adia} = \int dt \left(- \langle \Phi | \hat{H} | \Phi \rangle / \hbar \right) \quad (43)$$

This second Principle of Least Action involves the minimization of the action S_{adia} for arbitrary variations of the state vector, and this results in $|\Phi(t)\rangle$ satis-

fy the time-independent Schrodinger (or energy eigenvalue) equation (TISE). The variations of the state vector are subject to the constraint that it remains normalized to unity. This variational principle may be regarded as the fundamental principle for determining energy eigenstates, so its application to a specific case such as the BEC interferometry process is on firm ground. As before, the state vector is restricted in its possible variations (though remaining normalized to unity) to remaining in the form given by equation (31), and hence does not itself satisfy the TISE. What is obtained is a state vector which is an approximate solution to the TISE. However, the time-dependent mode functions that are obtained from the variational principle can not be obtained just by substituting for $|\Phi(t)\rangle$ in an energy eigenvalue equation. This variational approach has been applied in many other quantum physics problems - the derivation of the standard time-independent Gross-Pitaevskii equation for a single BEC being one example. It has already been applied to other BEC problems involving symmetrical double well potentials by Spekkens et al [31]. The application of the Least Action Principle to the adiabatic action to determine the mode functions and to the dynamic action to determine the amplitudes is designed to produce mode functions that would apply if the trapping potential were to change adiabatically, and to generate amplitudes that describe dynamical behavior in which the bosonic system may involve changing superpositions of different fragmented states. However, as will be seen below, the mode functions also reflect the possible way the BEC could fragment, with the more important fragmentation possibilities having greater influence in determining the mode functions. This is more realistic than determining mode functions based on some *a priori* assumption about fragmentation.

For fixed amplitudes $b_k(t)$ the action S_{adia} is a functional of modes $\phi_i(r, t)$. The orthogonality and normalization constraints in equation (15) for time τ may be written in terms of the functionals $G_\tau^{kl}[\phi_i, \phi_i^*]$, which are required to equal δ_{kl} . Thus

$$G_\tau^{kl}[\phi_i, \phi_i^*] = \int dt \int dr \phi_k^*(r, t) \phi_l(r, t) \delta(t - \tau) = \delta_{kl} \quad (44)$$

The action S_{adia} is minimized for arbitrary variation of the modes subject to the orthonormality constraints. The functional derivatives of the action S_{adia} plus the sum, integral of the constraints G_τ^{kl} each weighted with Lagrange multipliers $N\mu_{kl}(\tau)/\hbar$ are equated to zero. Thus we have:

$$\frac{\delta}{\delta \phi_i^*} \Delta S_{adia}[\phi_i, \phi_i^*] = \frac{\delta}{\delta \phi_i} \Delta S_{adia}[\phi_i, \phi_i^*] = 0 \quad (45)$$

$$\begin{aligned} \Delta S_{adia}[\phi_i, \phi_i^*] &= S_{adia}[\phi_i, \phi_i^*] + \\ &+ \sum_{kl} \int d\tau \frac{N\mu_{kl}(\tau)}{\hbar} G_\tau^{kl}[\phi_i, \phi_i^*] \end{aligned} \quad (46)$$

The Lagrange multipliers associated with the mode orthonormalization constraints form a Hermitian matrix of generalized chemical potentials $\mu_{ij}(t)$. The

key equations obtained for the modes $\phi_i(r, t)$ are coupled generalized Gross-Pitaevskii equations and are given below as equation (48). These equations are time-independent in that no time differentiation of the mode functions is involved, but they are time-dependent because the mode functions are time-dependent due to the presence of the time-dependent trapping potential $V(\mathbf{r}, t)$.

The coupled amplitude equations obtained are

$$i\hbar \frac{\partial b_k}{\partial t} = \sum_l (H_{kl} - \hbar U_{kl}) b_l \quad (k = -N/2, \dots, N/2). \quad (47)$$

These $N + 1$ equations (47) describe the system dynamics as it evolves amongst the possible fragmented states. The equations are similar to the standard amplitude equations obtained from matrix mechanics. In these equations the matrix elements H_{kl} , U_{kl} depend on the mode functions $\phi_i(r, t)$. Detailed expressions for H_{kl} , U_{kl} are given in Appendix 6. The matrix elements H_{kl} are in fact the matrix elements of the Hamiltonian \hat{H} in equation (13) between the fragmented states $|k\rangle$, $|l\rangle$. The matrix elements U_{kl} are elements of the so-called rotation matrix, and allow for the time dependence of the mode functions.

The coupled equations obtained for the two modes are

$$\begin{aligned} N \sum_j \mu_{ij} \phi_j &= \sum_j X_{ij} \left(-\frac{\hbar^2}{2m} \sum_{\mu=x,y,z} \partial_\mu^2 \phi_j + V \phi_j \right) \\ &+ g \sum_{jmn} Y_{ijmn} \phi_j^* \phi_m \phi_n \quad (i = 1, 2). \end{aligned} \quad (48)$$

These two equations (48) describe the adiabatic behavior of the two modes. The equations are coupled generalized Gross-Pitaevskii equations, rather than the usual single mode Gross-Pitaevskii equation [28], [29]. The coefficients X_{ij} , Y_{ijmn} depend quadratically on the amplitudes $b_k(t)$. The X_{ij} are $\sim N$, and the Y_{ijmn} are $\sim N^2$. Detailed expressions for X_{ij} , Y_{ijmn} are given in Appendix 6. The quantities μ_{ij} form a 2×2 Hermitian matrix to be referred to as the chemical potential matrix. Together the combined set of equations for the amplitudes and modes form a self-consistent set - neither the amplitude equations nor the generalized Gross-Pitaevskii equations can be solved independently of the other. This self-consistent feature is absent from most other treatments of BEC dynamics - the fragmentation behavior is often studied assuming that the modes are known in advance and considered fixed, whilst the mode functions are often calculated assuming some specific fragmentation, such as having half the bosons in each well. In the present work, the generalized Gross-Pitaevskii equations reflect the relative importance of all the possible fragmentations of the N bosons into the two modes.

The energy E of the bosonic system can also be expressed in terms of the mode functions $\phi_i(\mathbf{r}, t)$ and amplitudes $b_k(t)$. We find that

$$E = \langle \Phi(t) | \hat{H} | \Phi(t) \rangle \quad (49)$$

$$= \sum_{ij} X_{ij} \int d\mathbf{r} \phi_i^* \left(-\frac{\hbar^2}{2m} \sum_{\mu=x,y,z} \partial_\mu^2 + V \right) \phi_j + \frac{g}{2} \sum_{ijmn} Y_{ijmn} \int d\mathbf{r} \phi_i^* \phi_j^* \phi_m \phi_n. \quad (50)$$

As can be seen, the energy also depends on coefficients X_{ij} , Y_{ijmn} .

The chemical potential μ is defined as the derivative of the energy with respect to the boson number, and roughly gives the change in energy if one boson is added to the system. By writing $X_{ij} = x_{ij}^{(1)} N + O(N^0)$ and $Y_{ijmn} = y_{ijmn}^{(2)} N^2 + O(N^1)$ an expression for the chemical potential can be obtained using equations (50), (48). Thus we have

$$\mu = \frac{\partial E}{\partial N} \quad (51)$$

$$= \sum_i \mu_{ii} + O(N^0). \quad (52)$$

This result shows that the μ_{ij} form a generalized chemical potential matrix, the trace of which is the chemical potential.

The initial conditions for the amplitudes in the case where all the bosons are in mode ϕ_1 will be

$$b_k(0) = \delta_{k, -\frac{N}{2}}. \quad (53)$$

In this case only non-zero coefficients are

$$X_{11}(0) = N \quad Y_{1111}(0) = N(N-1), \quad (54)$$

and all the chemical potential matrix elements all zero except for μ_{11} . We find that the mode function $\phi_1(\mathbf{r}, 0)$ at time zero will then satisfy a single Gross-Pitaevskii equation of the form

$$\mu_{11} \phi_1 = -\frac{\hbar^2}{2m} \sum_{\mu=x,y,z} \partial_\mu^2 \phi_1 + V \phi_1 + g(N-1) |\phi_1|^2 \phi_1. \quad (55)$$

This result is the expected one for the case where all bosons are in mode ϕ_1 . The other mode function $\phi_2(\mathbf{r}, 0)$ is chosen by orthogonality.

The regime of validity for the present two-mode theory is determined using the criteria that the mean field energy $N g |\phi|^2$ is small compared to trap phonon energy $\hbar\omega_0$ [36], and the temperature T is much smaller than the transition temperature T_c . Applying these criteria lead to conditions on the boson number N and the temperature T

$$N \ll \frac{a_0}{a_s} \quad (56)$$

$$T \ll 0.94 N^{1/3} \frac{\hbar\omega_0}{k_B}, \quad (57)$$

where $a_0 = \sqrt{\hbar/2m\omega_0}$ is the harmonic oscillator vibrational amplitude. For Rb⁸⁷ with $a_s = 5$ nm, $a_0 = 1$ μ m, $\omega_0 = 2\pi.58$ s⁻¹, find $N \ll 2.10^2$ and $T \ll 15.4$ nK. Evidently the boson system can not be too large, nevertheless these conditions are realizable. Boson detection would be facilitated using metastable He⁴ to form the BEC.

4 Numerical Studies

Numerical solutions for the amplitude and generalized Gross-Pitaevski equations (47), (48) involve representing the amplitudes on a time grid and the mode functions on a space-time grid. The calculations would be facilitated by introducing dimensionless units for space and time based on harmonic oscillator units.

If there are N_T time points and N_{SX}, N_{SY}, N_{SZ} space points for each of the three space dimensions respectively, then the amplitudes and the mode functions will require $(N+1)N_T$ and $2N_T N_{SX} \cdot N_{SY} \cdot N_{SZ}$ complex values respectively - in all $N_T(N+1+2N_{SX} \cdot N_{SY} \cdot N_{SZ})$ values. The chemical potential matrix would also require another $4N_T$ values. Initial studies will be for the case where the splitting is essentially in one direction (Z), with the system tightly trapped in the two transverse (X, Y) directions. In this case it may be sufficient to take $N_{SX} = N_{SY} = 10$ and $N_{SZ} = 10^3$. With $N_T = 10^3$ systems with up to about $N = 10^5$ bosons would require about 3×10^8 values if all time or space-time values for amplitudes, mode functions, chemical potentials were to be stored in the computer.

Two possible approaches to carrying out the numerical studies are as follows. Both involve an iterative process. These may be referred to as: (a) Time evolution method (b) Matrix method

4.0.1 Time evolution method of solution

First Step:

1. Assume the amplitudes $b_k(t)$, the mode functions $\phi_i(\mathbf{r}, t)$ and an initial choice of their time derivatives $\partial_t \phi_i(\mathbf{r}, t)$ are known at time t
2. Calculate the spatial derivatives of the mode functions via

$$\partial_\mu \phi_i(\mathbf{r}, t) \simeq (\phi_i(\mathbf{r} + \Delta \mathbf{r}_\mu, t) - \phi_i(\mathbf{r}, t)) / \Delta r_\mu \quad (58)$$

3. Calculate the $H_{kl}(t)$ from (71) using equations (63), (64) for $\widetilde{W}_{ij}(\mathbf{r}, t)$ and $\widetilde{V}_{ijmn}(\mathbf{r}, t)$ and calculate $U_{kl}(t)$ from (68) using (65) for $\widetilde{T}_{ij}(\mathbf{r}, t)$
4. Use the approximation for small Δt

$$b_k(t + \Delta t) \simeq b_k(t) + \frac{\Delta t}{i\hbar} \sum_l (H_{kl}(t) - \hbar U_{kl}(t)) b_l(t) \quad (59)$$

together with applying the normalization requirement (32) to determine the amplitudes $b_k(t + \Delta t)$ at time $t + \Delta t$

Second Step:

1. Calculate the $X_{ij}(t + \Delta t)$ and $Y_{ij\ mn}(t + \Delta t)$ at time $t + \Delta t$ from equations (72), (73)
2. Solve the generalized GPE (48) for the mode functions $\phi_i(\mathbf{r}, t + \Delta t)$ at time $t + \Delta t$

Third Step:

1. Improve the values of the time derivatives $\partial_t \phi_i(\mathbf{r}, t)$ at time t via the expression
$$\partial_t \phi_i(\mathbf{r}, t) \simeq (\phi_i(\mathbf{r}, t + \Delta t) - \phi_i(\mathbf{r}, t)) / \Delta t \quad (60)$$
2. With the new $\partial_t \phi_i(\mathbf{r}, t)$ at time t go back to the first step and iterate the process until these time derivatives converge
3. The final $\partial_t \phi_i(\mathbf{r}, t)$ may then be used as the initial choice for $\partial_t \phi_i(\mathbf{r}, t + \Delta t)$ at time $t + \Delta t$

Fourth Step:

1. As the amplitudes $b_k(t + \Delta t)$, the mode functions $\phi_i(\mathbf{r}, t + \Delta t)$ and an initial choice of their time derivatives $\partial_t \phi_i(\mathbf{r}, t + \Delta t)$ are now known at time $t + \Delta t$ we can go back to the first step and repeat the process to obtain the results at time $t + 2\Delta t$
2. The process continues for further time points $t + 3\Delta t, t + 4\Delta t, t + 5\Delta t, \dots$

Fifth Step:

1. The process begins with $t = 0$ using the initial amplitudes $b_k(0)$ given by (53) and mode functions $\phi_i(\mathbf{r}, 0)$ obtained from (55) and orthogonality. The initial choice of time derivatives at $t = 0$ may be assumed to be zero, as the process will correct this initial arbitrary choice.

The advantage of the time evolution method is that the values for the amplitudes, mode functions, their spatial and time derivatives and the chemical potentials need only be retained at two times t and $t + \Delta t$, thus only $2(N + 5 + 10N_{SX}.N_{SY}.N_{SZ})$ simultaneous values would be stored. If we take $N_{SX} = N_{SY} = 10$ and $N_{SZ} = 10^3$, then systems with up to about $N = 10^5$ bosons would require about 2×10^6 values to be simultaneously stored in the computer.

4.0.2 Matrix method of solution

First Step:

1. Assume a solution for the amplitudes b_k as functions of time
2. Calculate the X_{ij} and $Y_{ij\,mn}$ as functions of time
3. Solve the generalized GPE (48) for the mode functions ϕ_i as space-time functions via non-linear matrix methods

Second Step:

1. Using equations (58), (60) to obtain the spatial and time derivatives, calculate the H_{kl} and U_{kl} as functions of time
2. Solve the amplitude equations (47) for the amplitudes b_k as functions of time via matrix methods.

Third Step:

1. Repeat the process until the solutions for the mode functions and amplitudes converge.

This approach represents the space-time values and time values of the mode functions and amplitudes in a column vector and then the non-linear equations for this vector obtained from equations (47), (48) are solved via matrix methods. Here the values for the amplitudes, mode functions, their spatial and time derivatives and the chemical potentials need only be retained at all times, which as we have seen would require about 3×10^8 values for systems with up to about $N = 10^5$ bosons.

5 Summary

Using the two-mode approximation and treating the N bosons as a giant spin system, a theory of BEC interferometry has been developed by applying the Principle of Least Action to a variational form for the quantum state which allows for the possibility that the BEC fragments into two, as well as for the outcome where only a single BEC ever occurs. The amplitudes for the possible fragmented states describe the dynamics and are determined from the dynamic action. The two spatial mode functions describe the adiabatic behavior and are obtained from the adiabatic action.

Self-consistent coupled equations have been obtained for the state amplitudes and the modes, the former being in the form of standard matrix mechanics equations, the latter equations being a generalization of the time independent Gross-Pitaevskii equations and which involve generalized chemical potentials. The self-consistent feature is that the mode functions are needed to determine

the Hamiltonian and rotation matrices that appear in the amplitude equations, whilst the amplitudes for possible fragmented states determine coefficients that appear in the generalized Gross-Pitaevskii equations for the modes. Unlike previous work, the mode equations reflect the relative importance of all the possible divisions or fragmentations of the bosons into two modes.

Numerical studies of these equations are planned, aimed at applications in future BEC interferometry experiments at Swinburne University of Technology involving a double well interferometer based on atom chips. Two approaches for carrying out these numerical studies have been outlined.

6 Appendix - Expressions for quantities in amplitude and mode equations

In the two-mode approximation the N boson system behaves like a giant spin system with spin quantum number $j = N/2$ and which can be described via angular momentum eigenstates $|\frac{N}{2}, k\rangle$, where $k = -N/2, \dots, +N/2$ is a magnetic quantum number which describes fragmented states of the bosonic system with $(\frac{N}{2} - k)$ bosons in mode $\phi_1(r, t)$ and $(\frac{N}{2} + k)$ bosons in mode $\phi_2(r, t)$. It is therefore not surprising that the basic equations will involve expressions arising from angular momentum theory. These are the quantities X_{kl}^{ij} and $Y_{kl}^{ij\ mn}$ which are defined as

$$\begin{aligned}
X_{kl}^{11} &= (\frac{N}{2}-k)\delta_{kl} & X_{kl}^{12} &= \{(\frac{N}{2}-k)(\frac{N}{2}+l)\}^{\frac{1}{2}}\delta_{k,l-1} \\
X_{kl}^{21} &= \{(\frac{N}{2}-l)(\frac{N}{2}+k)\}^{\frac{1}{2}}\delta_{l,k-1} & X_{kl}^{22} &= (\frac{N}{2}+k)\delta_{kl} \\
Y_{kl}^{1111} &= (\frac{N}{2}-k)(\frac{N}{2}-k-1)\delta_{kl} \\
Y_{kl}^{2222} &= (\frac{N}{2}+k)(\frac{N}{2}+k-1)\delta_{kl} \\
Y_{kl}^{1212} &= Y_{kl}^{1221} = Y_{kl}^{2112} = Y_{kl}^{2121} = (\frac{N}{2}-k)(\frac{N}{2}+k)\delta_{kl} \\
Y_{kl}^{1112} &= Y_{kl}^{1121} = (\frac{N}{2}-l)\{(\frac{N}{2}-k)(\frac{N}{2}+l)\}^{\frac{1}{2}}\delta_{k,l-1} \\
Y_{kl}^{1222} &= Y_{kl}^{2122} = (\frac{N}{2}+k)\{(\frac{N}{2}-k)(\frac{N}{2}+l)\}^{\frac{1}{2}}\delta_{k,l-1} \\
Y_{kl}^{1211} &= Y_{kl}^{2111} = (\frac{N}{2}-k)\{(\frac{N}{2}-l)(\frac{N}{2}+k)\}^{\frac{1}{2}}\delta_{l,k-1} \\
Y_{kl}^{2212} &= Y_{kl}^{2221} = (\frac{N}{2}+l)\{(\frac{N}{2}-l)(\frac{N}{2}+k)\}^{\frac{1}{2}}\delta_{l,k-1} \\
Y_{kl}^{1122} &= \{(\frac{N}{2}-l+1)(\frac{N}{2}-k)(\frac{N}{2}+l)(\frac{N}{2}+k+1)\}^{\frac{1}{2}}\delta_{k,l-2} \\
Y_{kl}^{2211} &= \{(\frac{N}{2}-k+1)(\frac{N}{2}-l)(\frac{N}{2}+k)(\frac{N}{2}+l+1)\}^{\frac{1}{2}}\delta_{l,k-2}.
\end{aligned} \tag{61}$$

The Hamiltonian and rotation matrix elements H_{kl} and U_{kl} that occur in the amplitude equations (47) involve spatial integrals involving the mode functions ϕ_1 and ϕ_2 . They are therefore functionals of the mode functions. The expressions depend also on the spatial and time derivatives of the mode functions through the quantities $\widetilde{W}_{ij}(\mathbf{r}, t)$, $\widetilde{V}_{ijmn}(\mathbf{r}, t)$ and $\widetilde{T}_{ij}(\mathbf{r}, t)$, where $(i, j, m, n = 1, 2)$, and which are defined by

$$\widetilde{W}_{ij}(\mathbf{r}, t) = \frac{\hbar^2}{2m} \sum_{\mu=x,y,z} \partial_{\mu}\phi_i^* \partial_{\mu}\phi_j + \phi_i^* V \phi_j \tag{63}$$

$$\widetilde{V}_{ijmn}(\mathbf{r}, t) = \frac{g}{2} \phi_i^* \phi_j^* \phi_m \phi_n \tag{64}$$

$$\widetilde{T}_{ij}(\mathbf{r}, t) = \frac{1}{2i} (\partial_t \phi_i^* \phi_j - \phi_i^* \partial_t \phi_j) \tag{65}$$

The rotation matrix elements U_{kl} ($-\frac{N}{2} \leq k, l \leq +\frac{N}{2}$) are given by

$$U_{kl} = \frac{1}{2i} [(\partial_t \langle k |) | l \rangle - \langle k | (\partial_t | l \rangle)] = U_{lk}^* \tag{66}$$

$$= \int d\mathbf{r} \widetilde{U}_{kl}(\phi_i, \phi_i^*, \partial_t \phi_i, \partial_t \phi_i^*). \tag{67}$$

In the expression (67) for the rotation matrix the quantity \tilde{U}_{kl} is

$$\tilde{U}_{kl} = \sum_{ij} X_{kl}^{ij} \tilde{T}_{ij}. \quad (68)$$

The result involves the angular momentum theory quantities X_{kl}^{ij} . Thus for the rotation matrix, space integrals of the mode functions and their time derivatives are involved.

The Hamiltonian matrix elements H_{kl} ($-\frac{N}{2} \leq k, l \leq +\frac{N}{2}$) are given by

$$H_{kl} = \langle k | \hat{H} | l \rangle = H_{lk}^* \quad (69)$$

$$= \int d\mathbf{r} \tilde{H}_{kl}(\phi_i, \phi_i^*, \partial_\mu \phi_i, \partial_\mu \phi_i^*). \quad (70)$$

In the expression (70) for the Hamiltonian matrix the quantity \tilde{H}_{kl} is a Hamiltonian density and is given by

$$\tilde{H}_{kl} = \sum_{ij} X_{kl}^{ij} \tilde{W}_{ij} + \sum_{ijmn} Y_{kl}^{ijmn} \tilde{V}_{ijmn}. \quad (71)$$

This result involves the angular momentum theory quantities X_{kl}^{ij} and Y_{kl}^{ijmn} . Thus for the Hamiltonian matrix, space integrals of the mode functions and their spatial derivatives are involved.

The coefficients X_{ij} and Y_{ijmn} ($i, j, m, n = 1, 2$) that occur in the generalized Gross-Pitaevskii equations (48) for the mode functions are quadratic functions of the amplitudes b_k ($-\frac{N}{2} \leq k, l \leq +\frac{N}{2}$)

$$X_{ij} = \sum_{k,l} b_k^* X_{kl}^{ij} b_l = X_{ji}^* \sim N \quad (72)$$

$$Y_{ijmn} = \sum_{k,l} b_k^* Y_{kl}^{ijmn} b_l = Y_{mnij}^* \sim N^2 \quad (73)$$

Note the Hermitian properties of these quantities and the N dependence of their order of magnitude.

7 Figure captions

Figure 1. The interferometer process. A trapping potential (shown in red) is changed from a single well into an asymmetric double well and back to a single well again. Initially all the bosons (shown as squares) are in the symmetric lowest mode of the single well, at the end of the process some bosons are in the antisymmetric first excited mode of the single well. Mode functions are depicted in pink and blue, and possible changes to the mode functions during the double well intermediate stage are shown.

Figure 2. Bosons in a symmetric double well trap showing possible fragmentation effects. For low barrier heights and small inter-well separation (as in

(a)) a single unfragmented BEC occurs, with all bosons in the symmetric mode delocalized between the two wells (Josephson phase). For the opposite situation (as in (b)) the BEC fragments into two, with half the bosons in localized modes in each well (Mott phase). Trap asymmetry is ignored.

Figure 3. Mode functions in asymmetric trapping potentials showing localization and delocalization effects in the double well regime. For the single well regime (a) the symmetric and antisymmetric two lowest modes are shown. For the double well regime with small asymmetry (b) two delocalized modes are shown, one approximately symmetric the other approximately antisymmetric. For the double well regime with large asymmetry (c) two localized modes are shown, each localized in a different well. Boson-boson interactions are ignored.

Figure 4. BEC interferometry as a quantum interference process. The case with $N = 9$ bosons initially in mode $\phi_1(r, 0)$ and $n = 1$ bosons finally transferred to mode $\phi_2(r, T)$ is shown. Two quantum pathways are present depending on whether the transfer occurs between $t = 0$ and $t = T/2$ or between $t = T/2$ and $t = T$.

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